

FIG. 1(a)

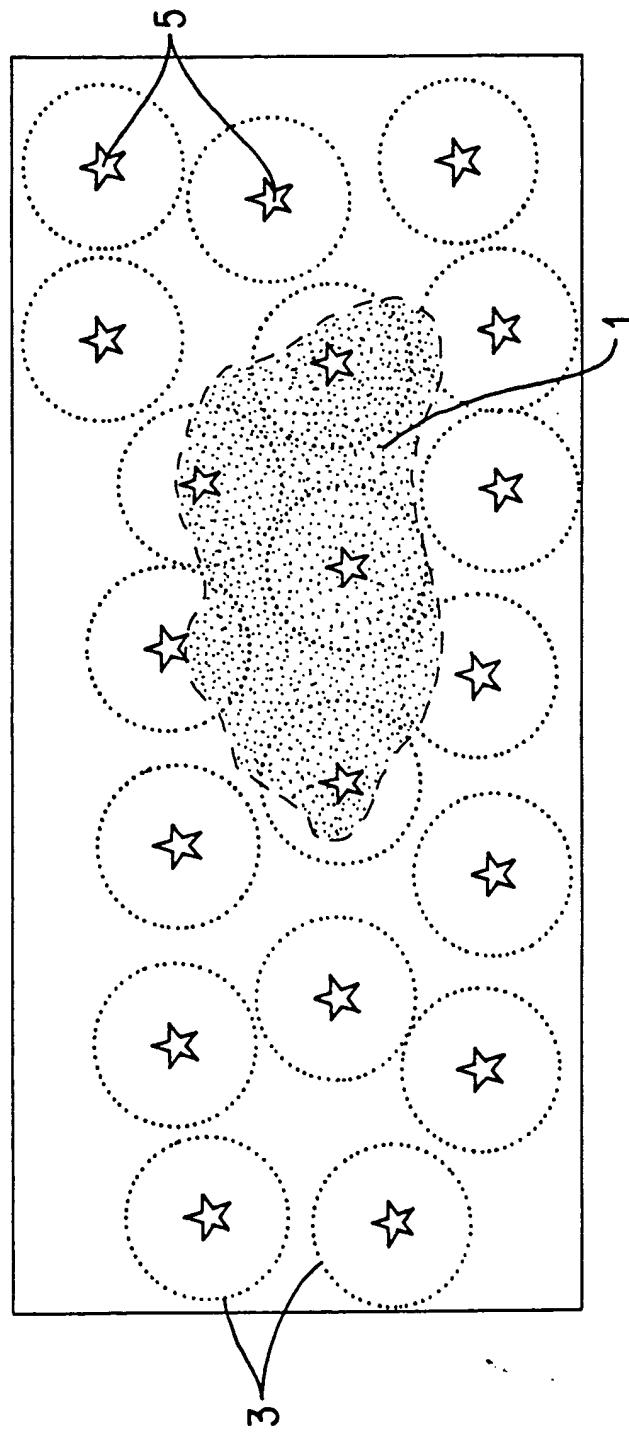


FIG. 1(b)

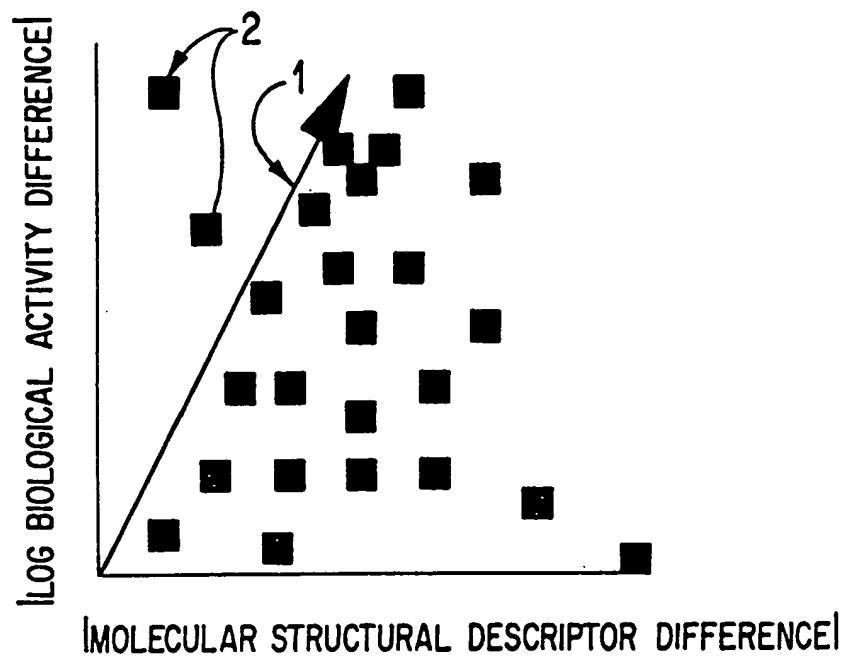


FIG. 2

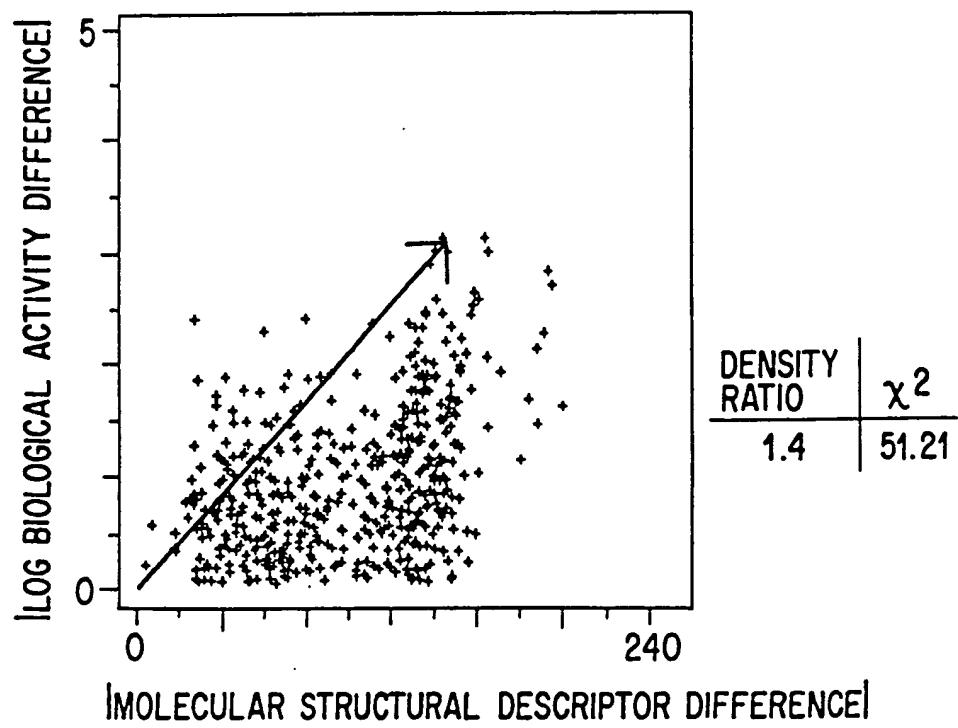
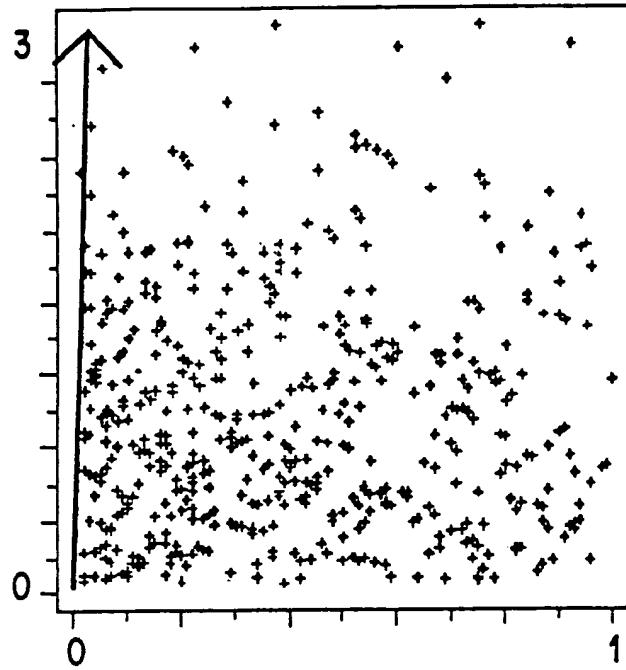


FIG. 3

LOG BIOLOGICAL ACTIVITY DIFFERENCE



DENSITY
RATIO

1.00

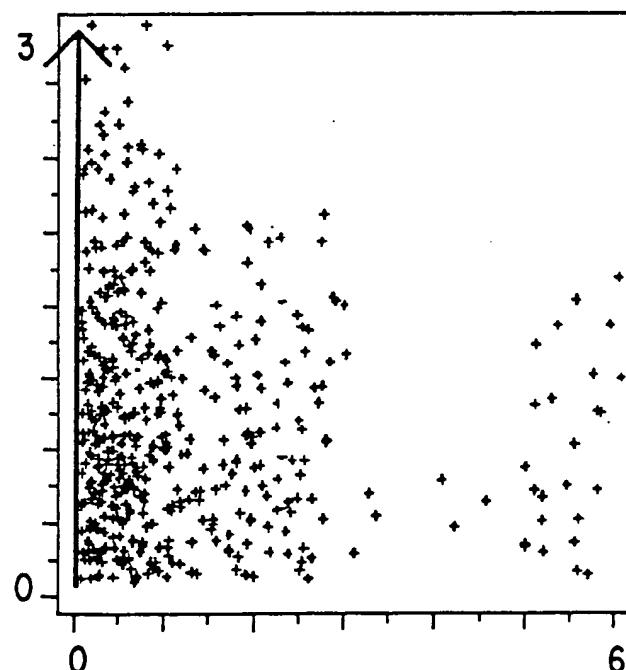
χ^2

0.00

RANDOM NUMBER DIFFERENCE

FIG. 4

LOG BIOLOGICAL ACTIVITY DIFFERENCE



DENSITY
RATIO

0.96

χ^2

0.46

(FORCE FIELD STRAIN ENERGY)/ATOM DIFFERENCE

FIG. 5

ATTACHED
TO CORE

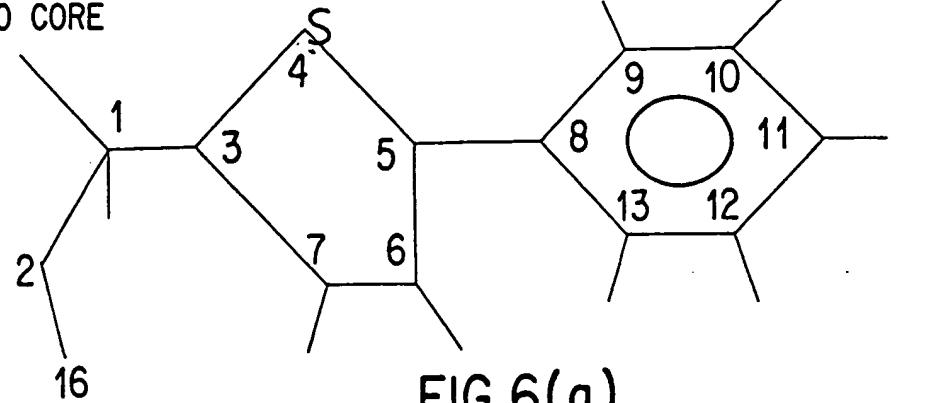


FIG. 6(a)

ATTACHED
TO CORE

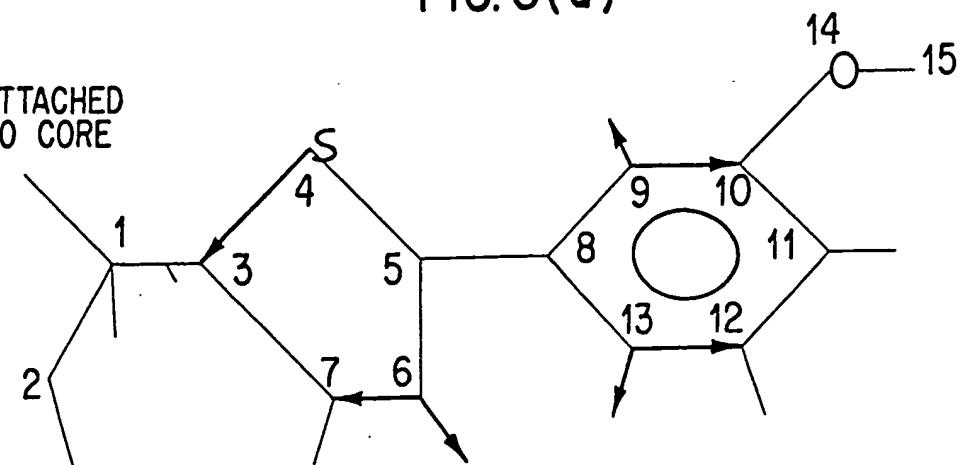


FIG. 6(b)

ATTACHED
TO CORE

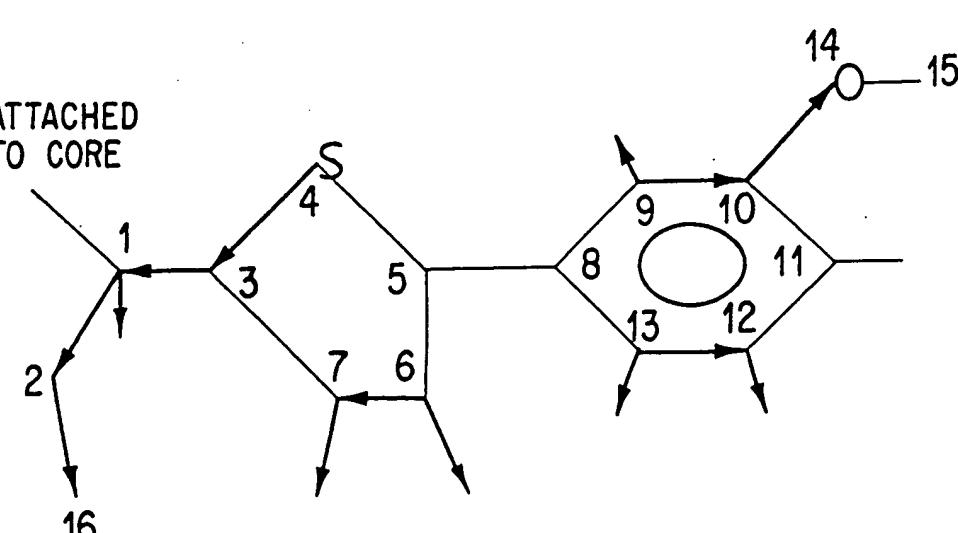


FIG. 6(c)

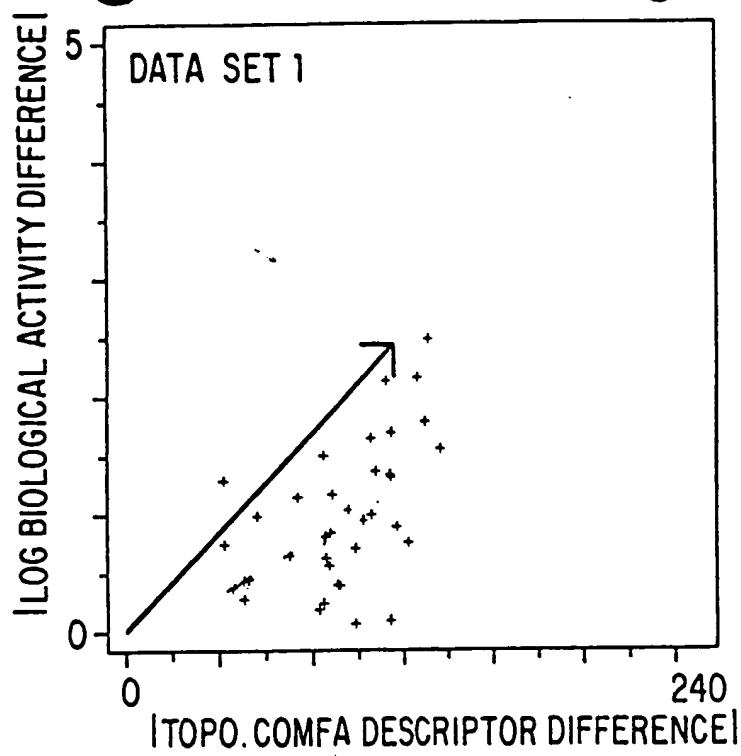


FIG.7(a)

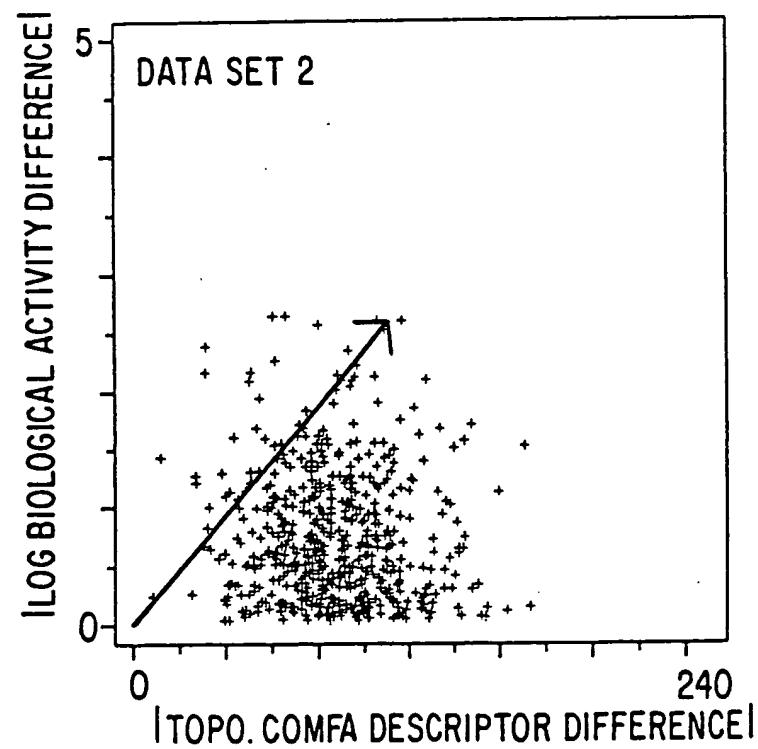


FIG.7(b)

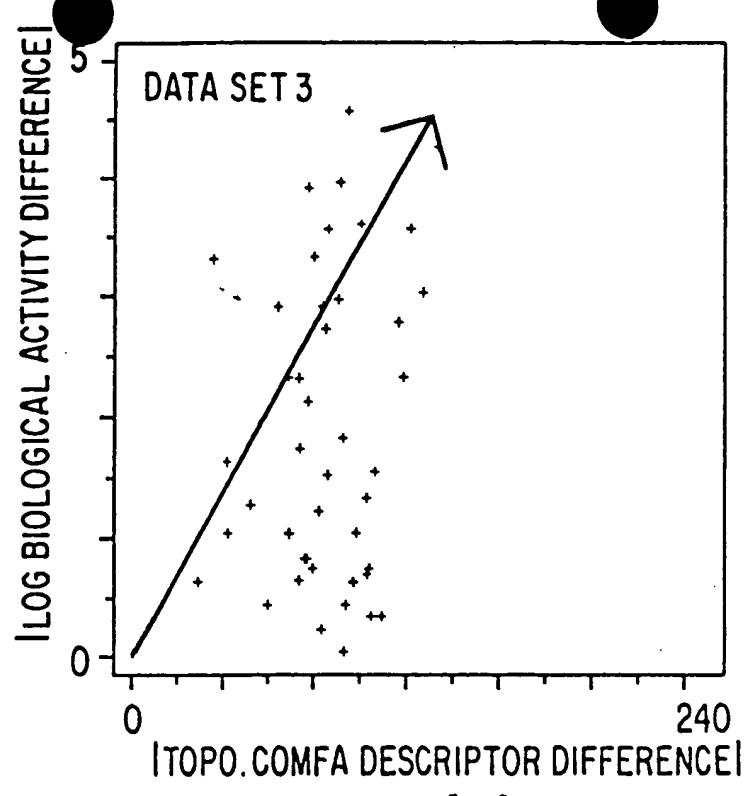


FIG. 7(c)

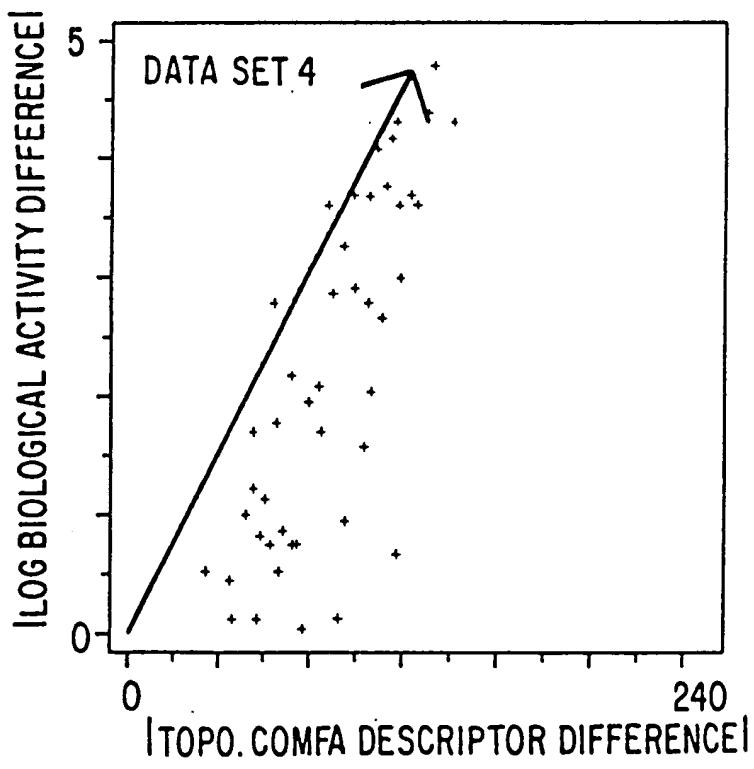


FIG. 7(d)

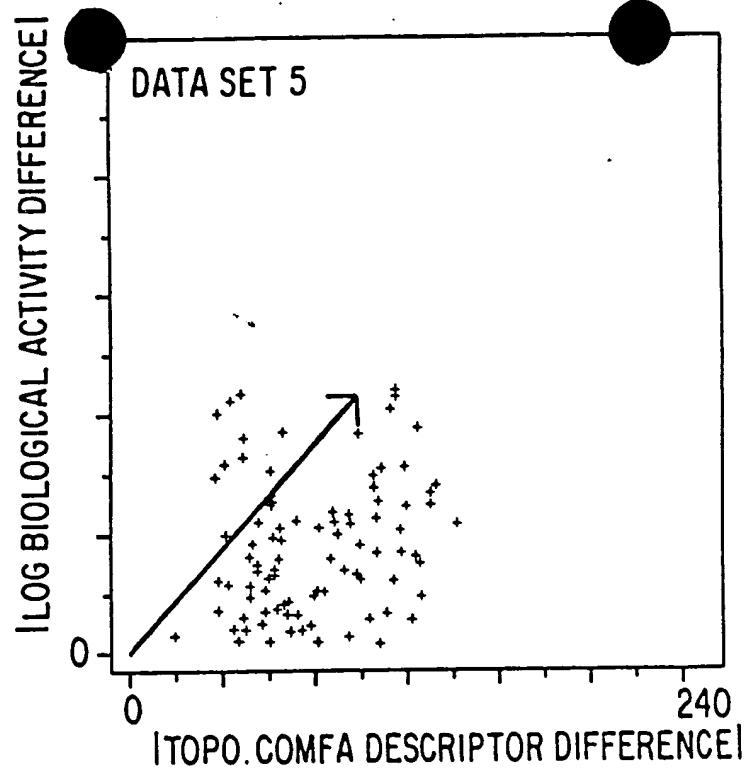


FIG.7(e)

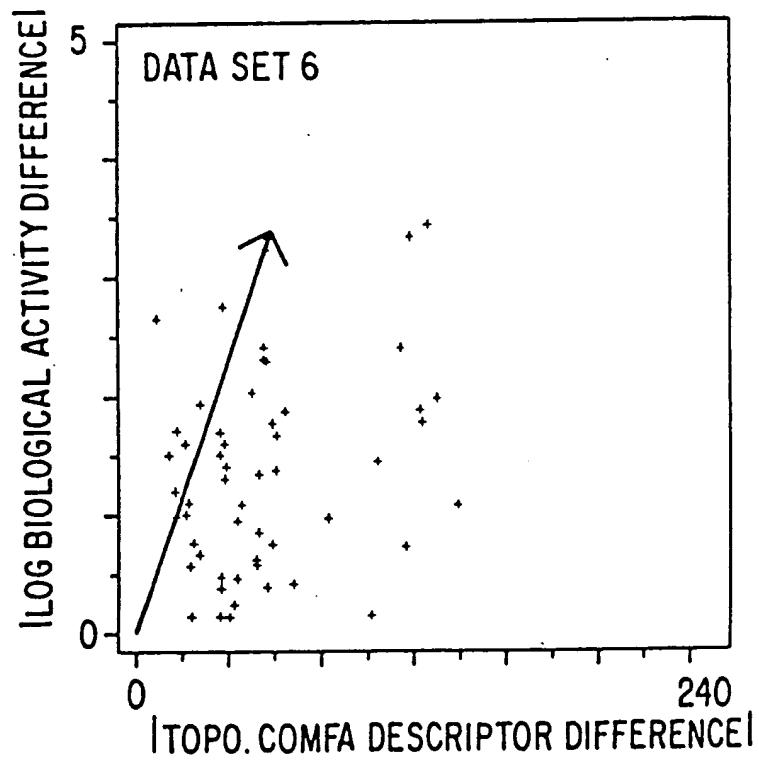


FIG.7(f)

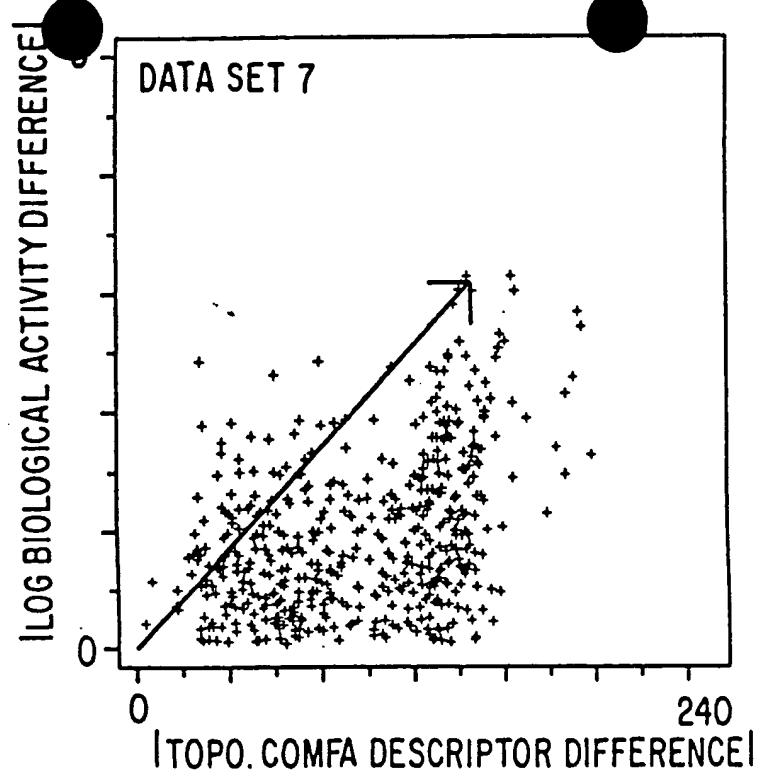


FIG.7(g)

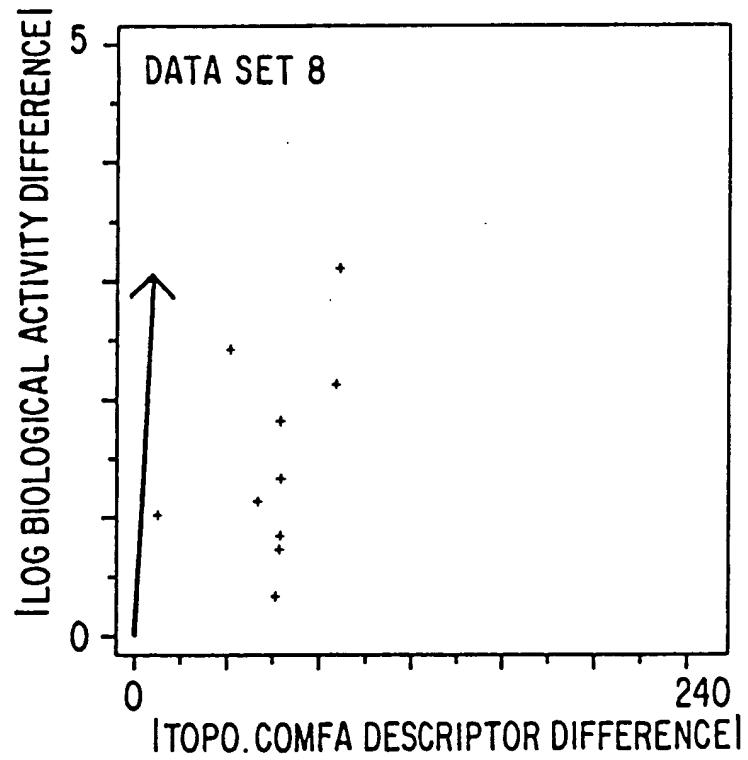


FIG.7(h)

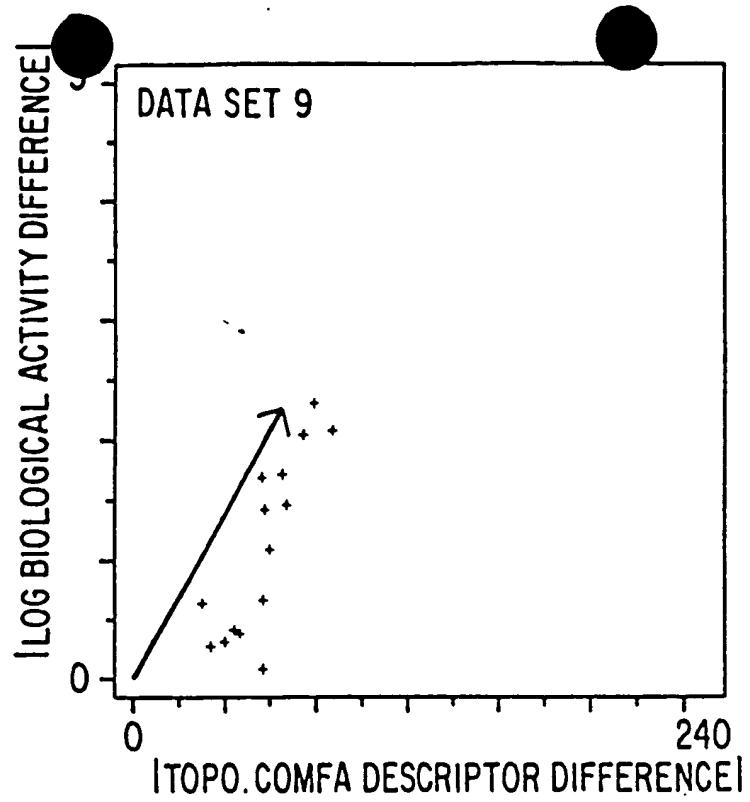


FIG.7(i)

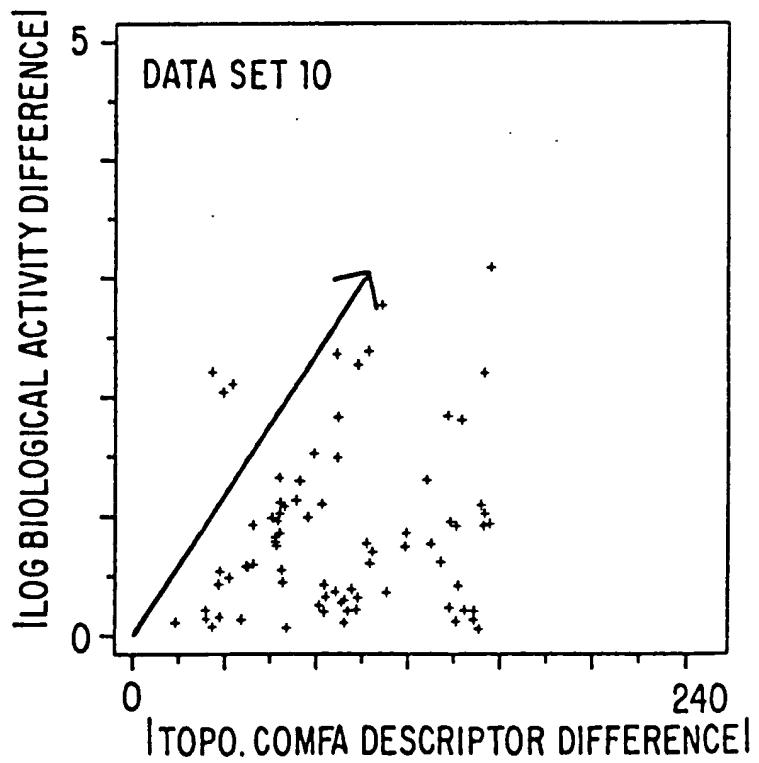


FIG.7(j)

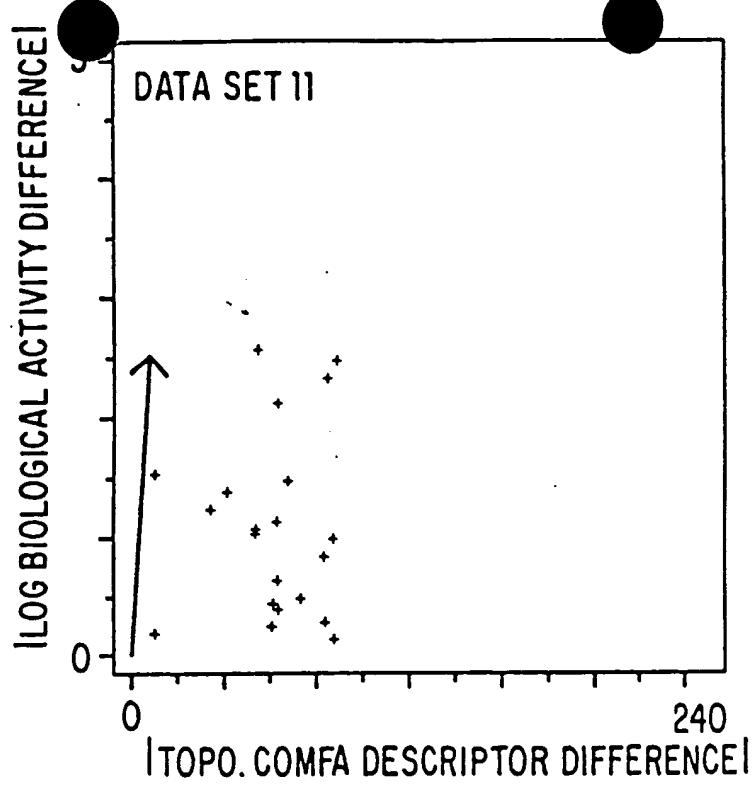


FIG.7(k)

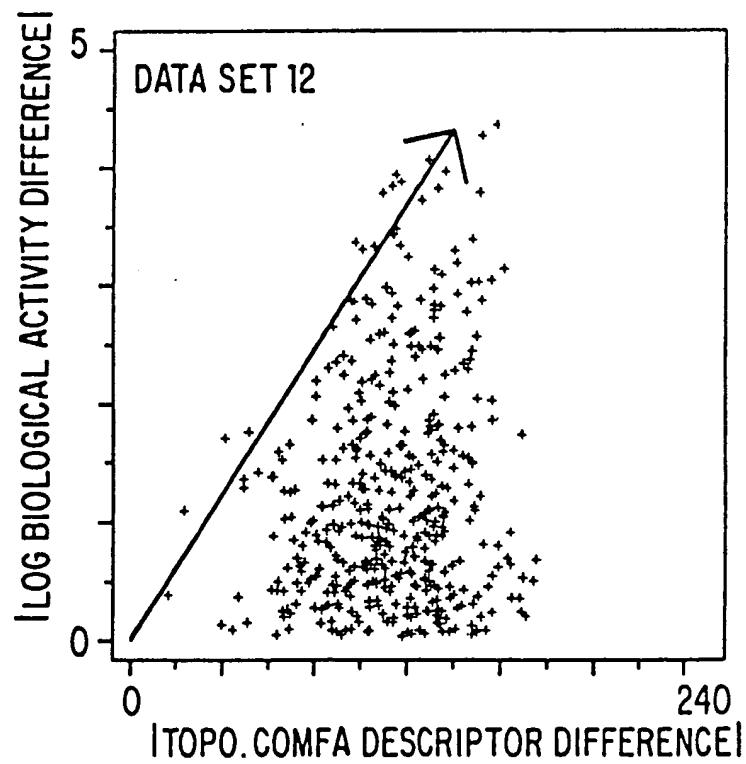


FIG.7(l)

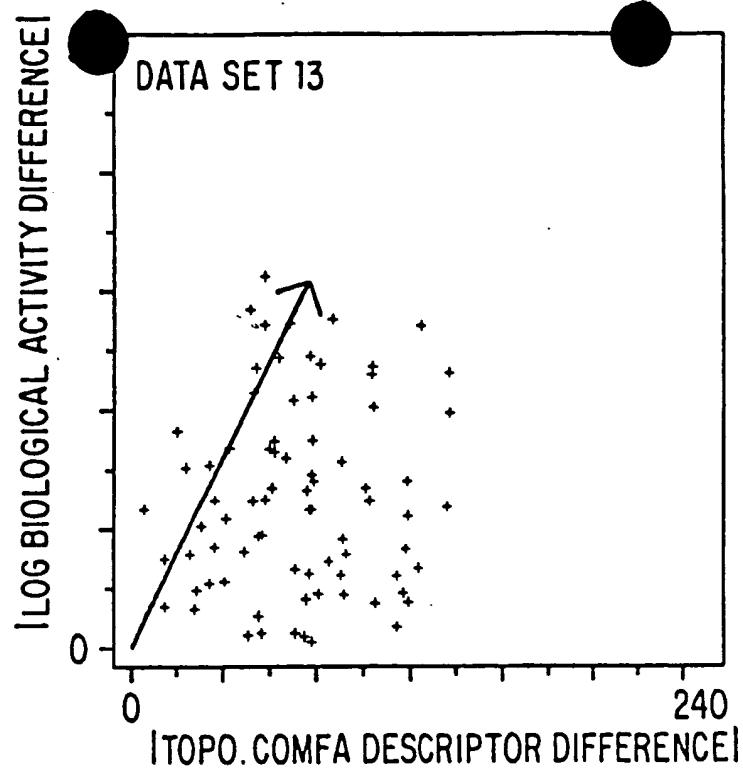


FIG. 7(m)

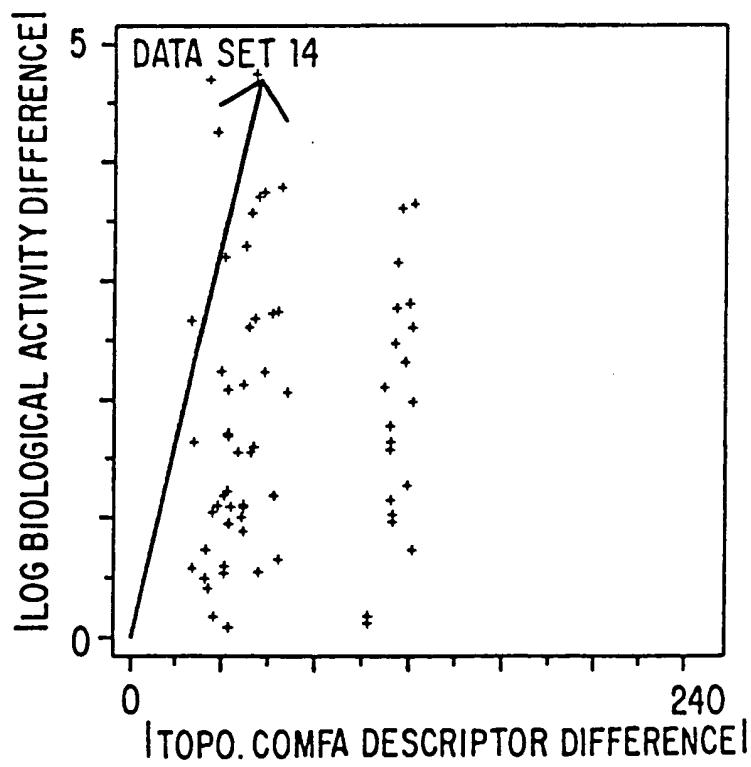


FIG. 7(n)

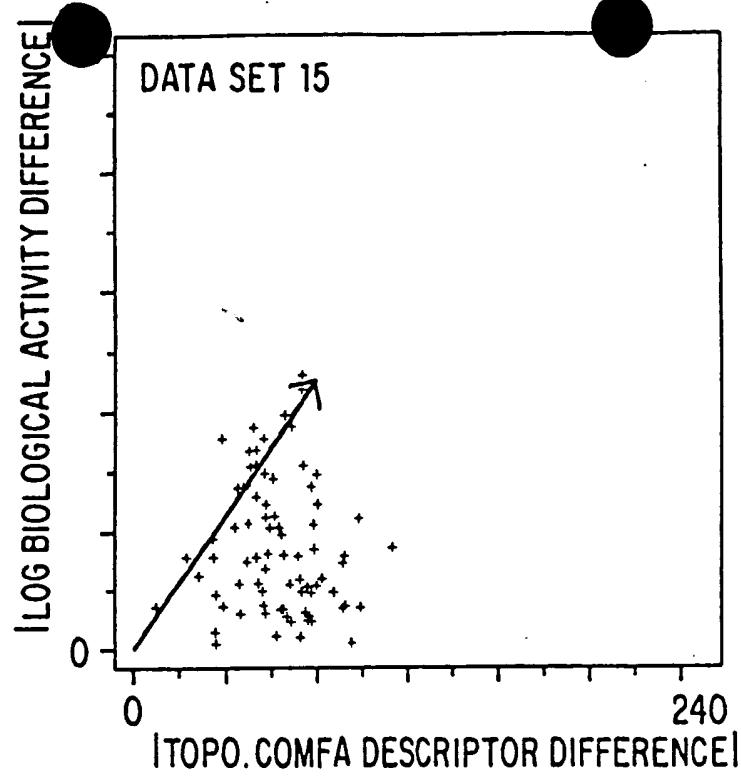


FIG.7(o)

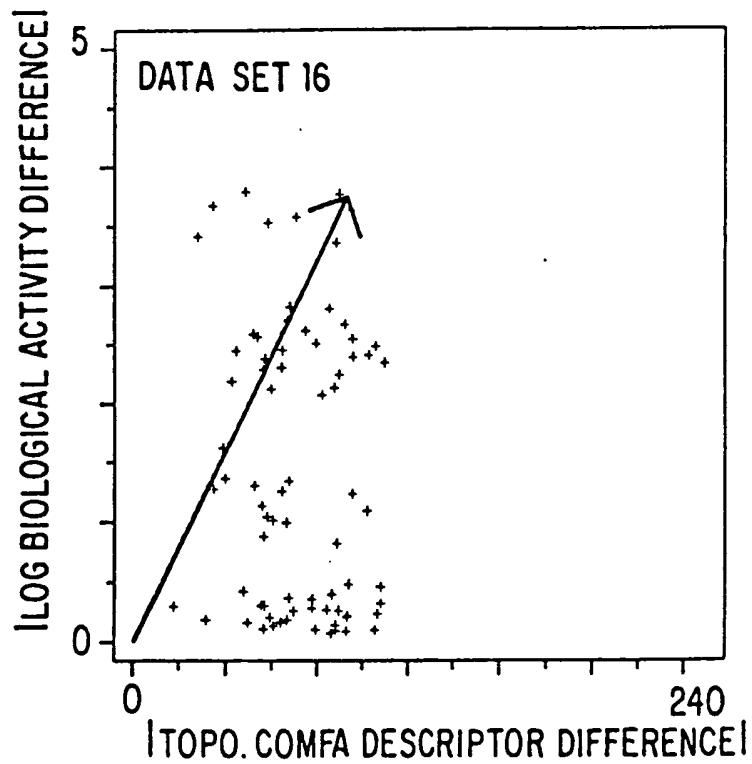
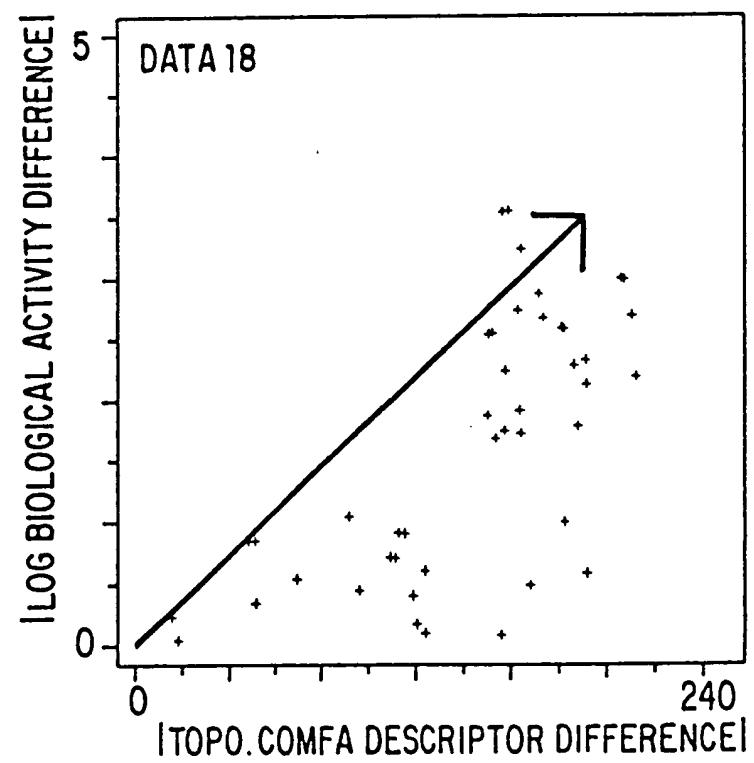
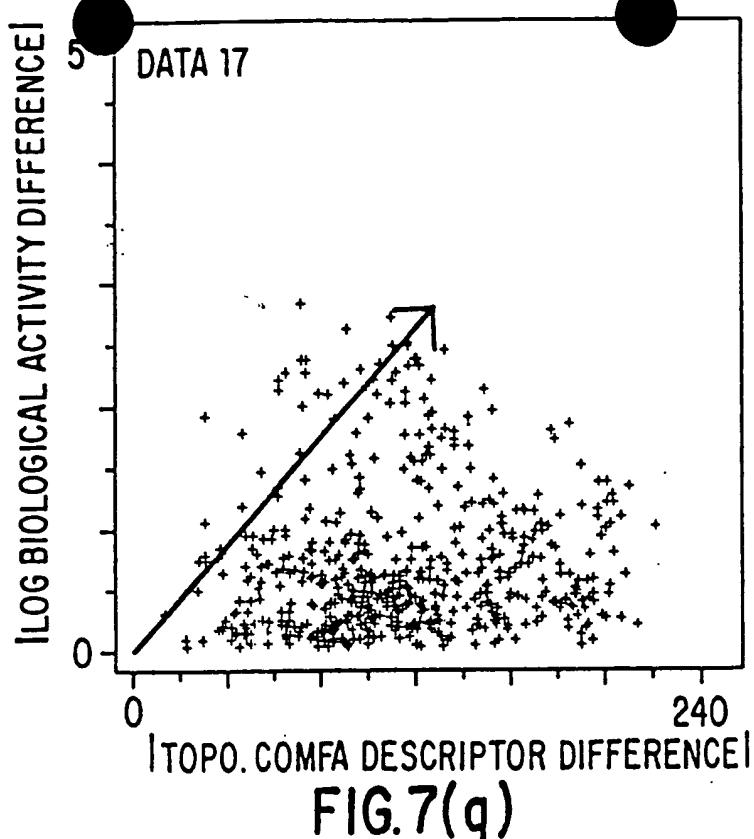
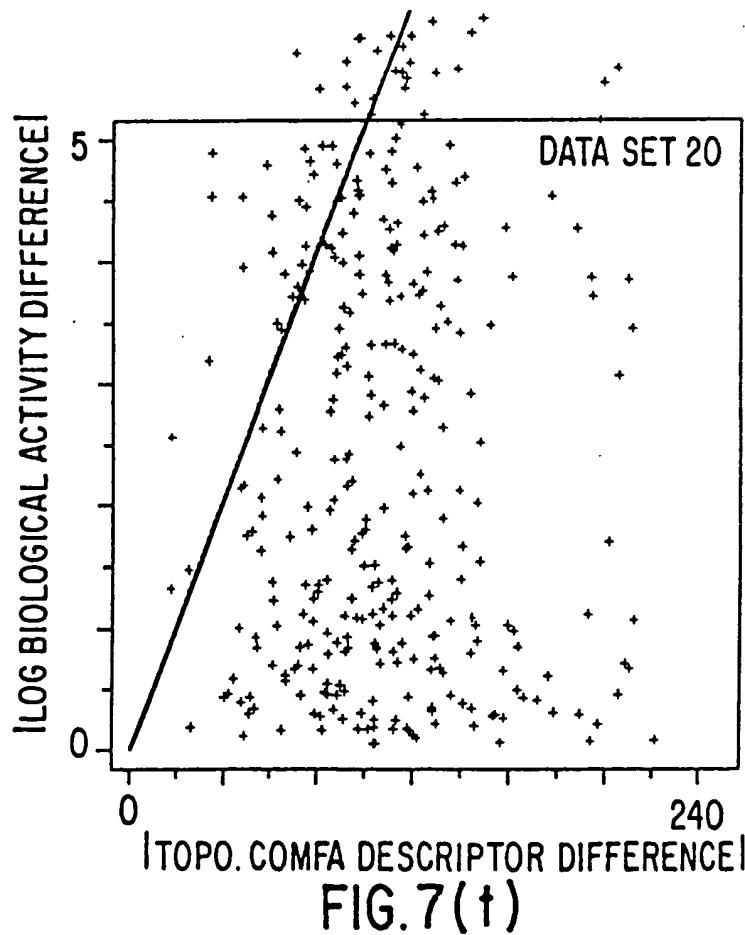
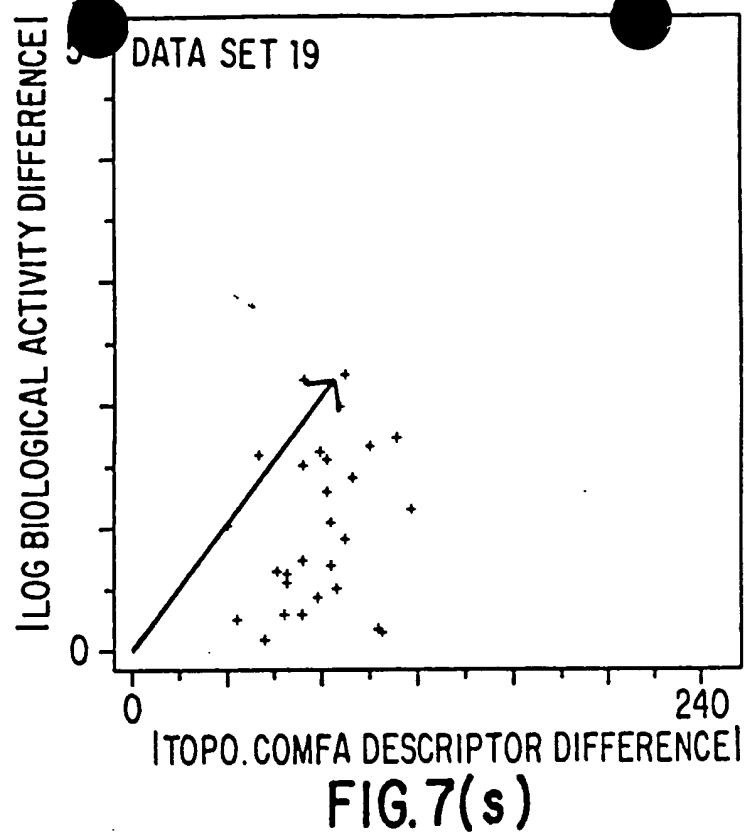
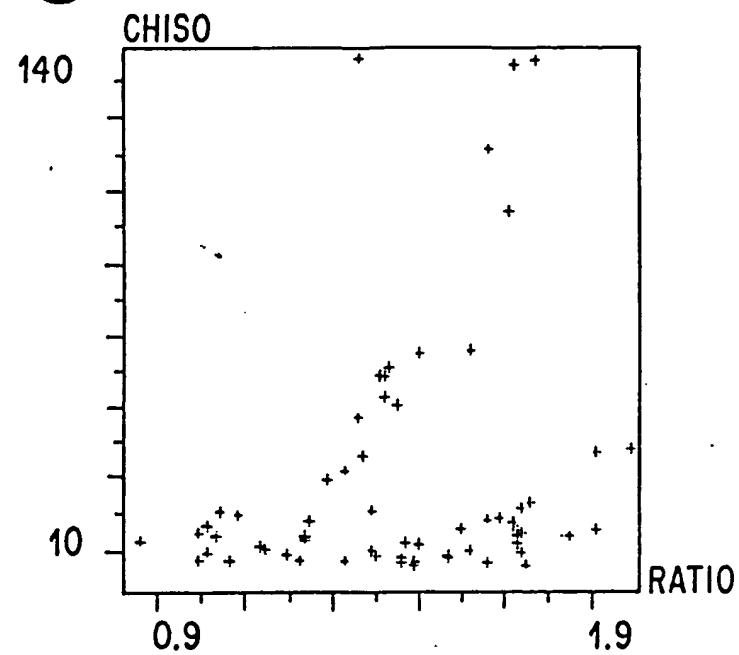


FIG.7(p)







↑
1.1

FIG. 8(a)

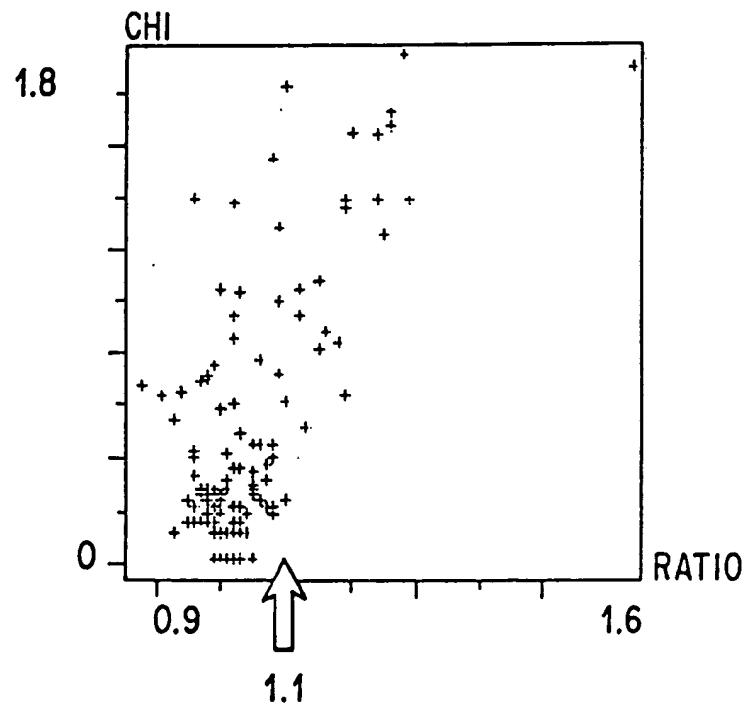


FIG. 8(b)

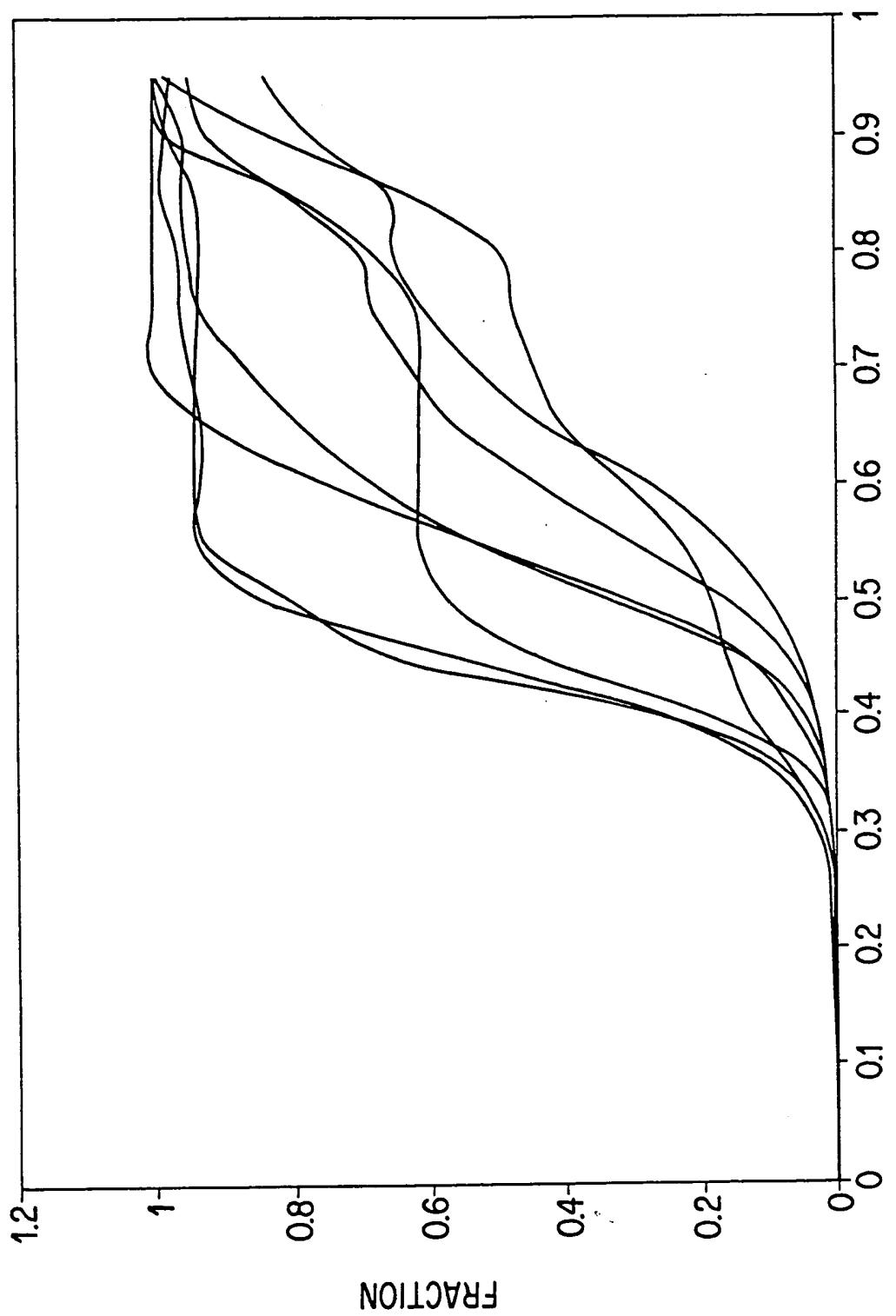
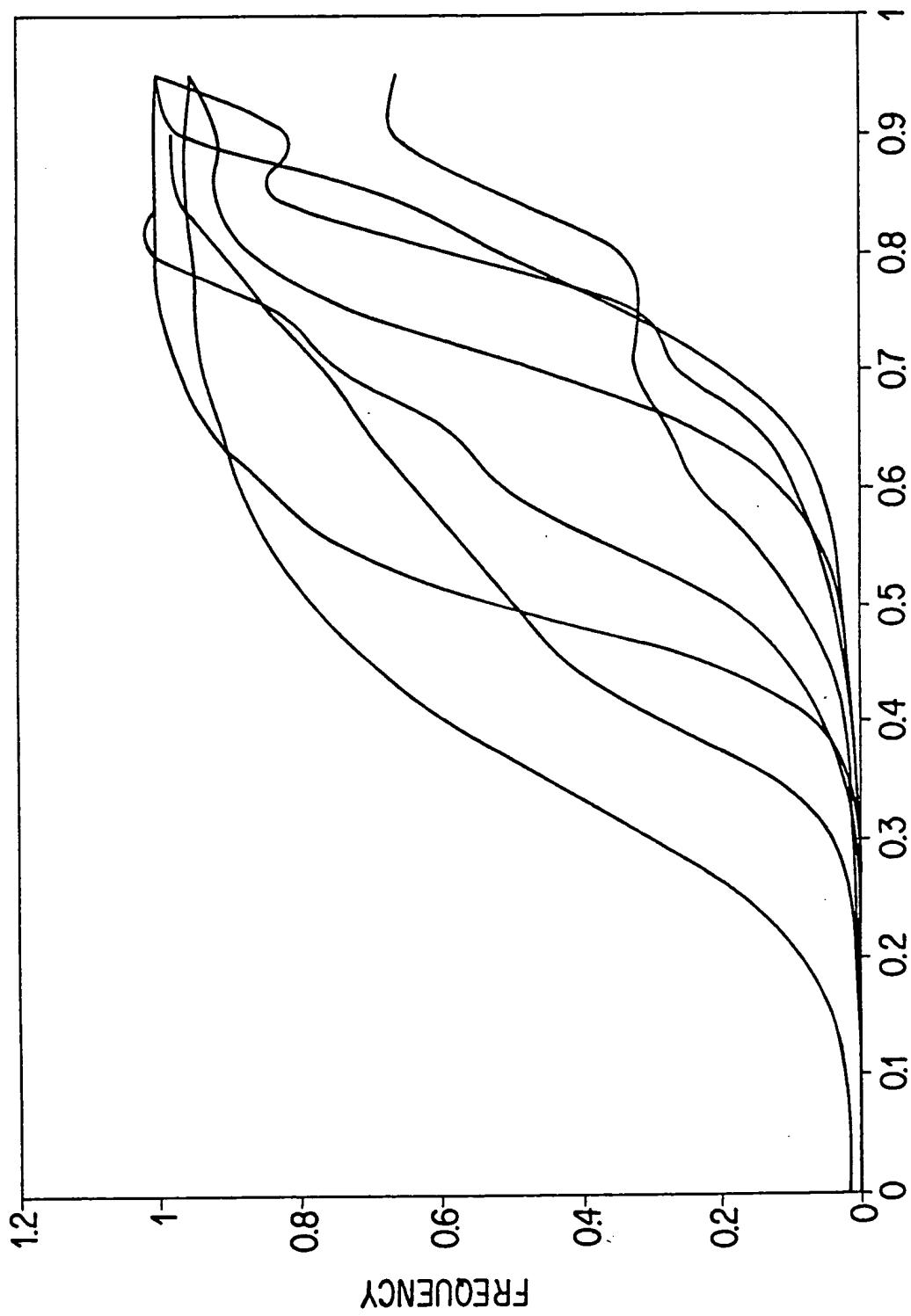
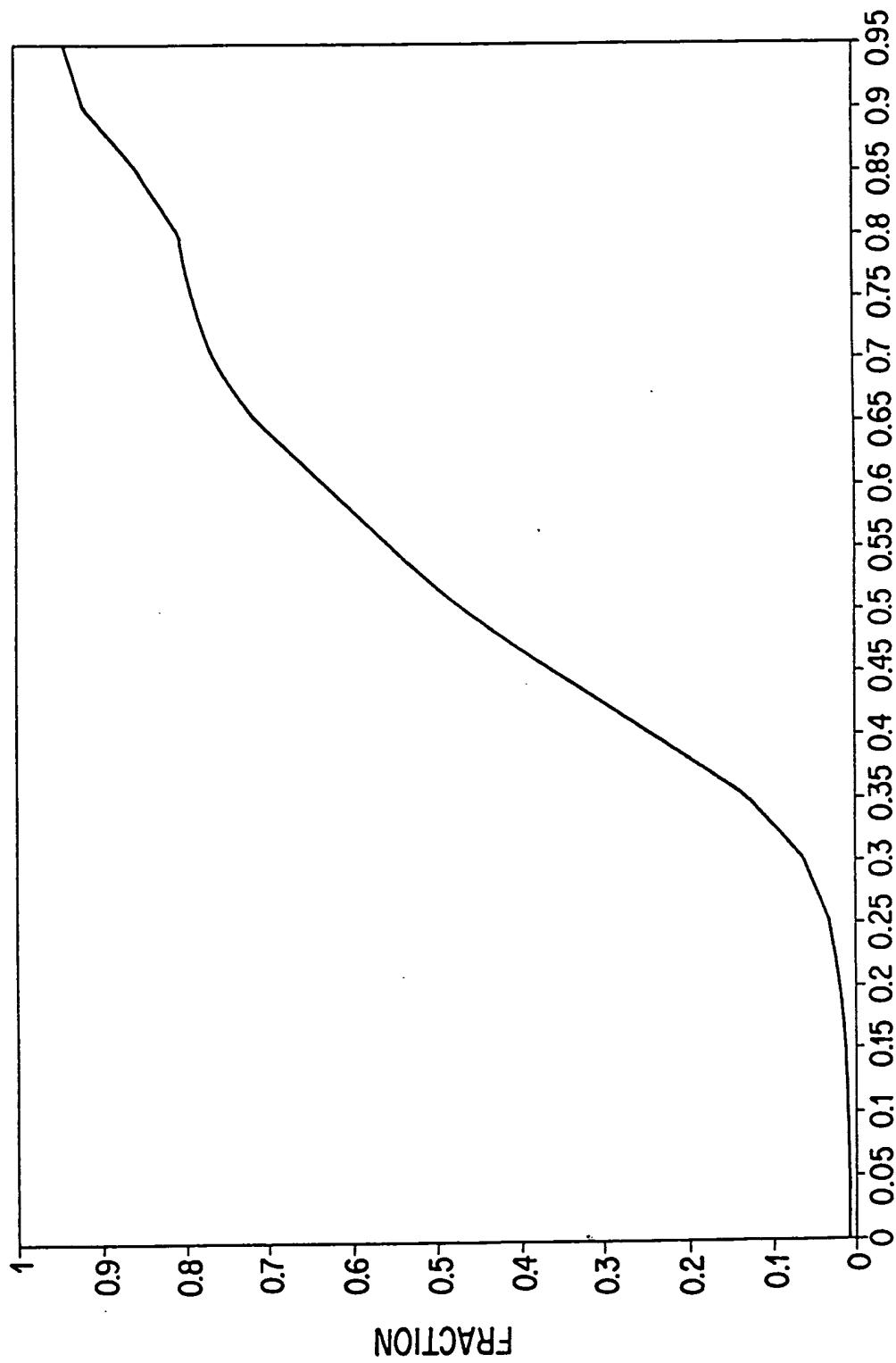


FIG. 9(a)

FIG. 9(b)





TANIMOTO

FIG. 9(c)

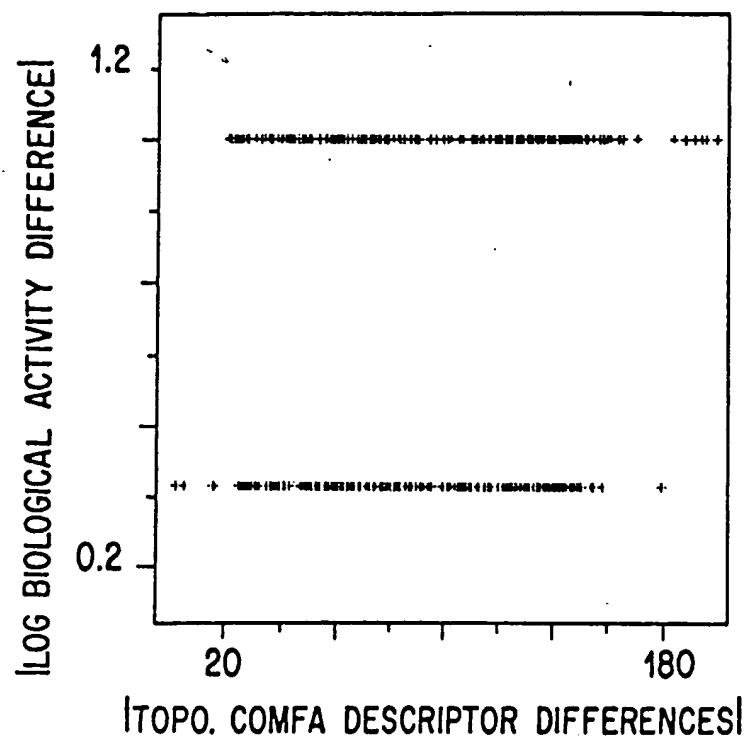


FIG.10(a)

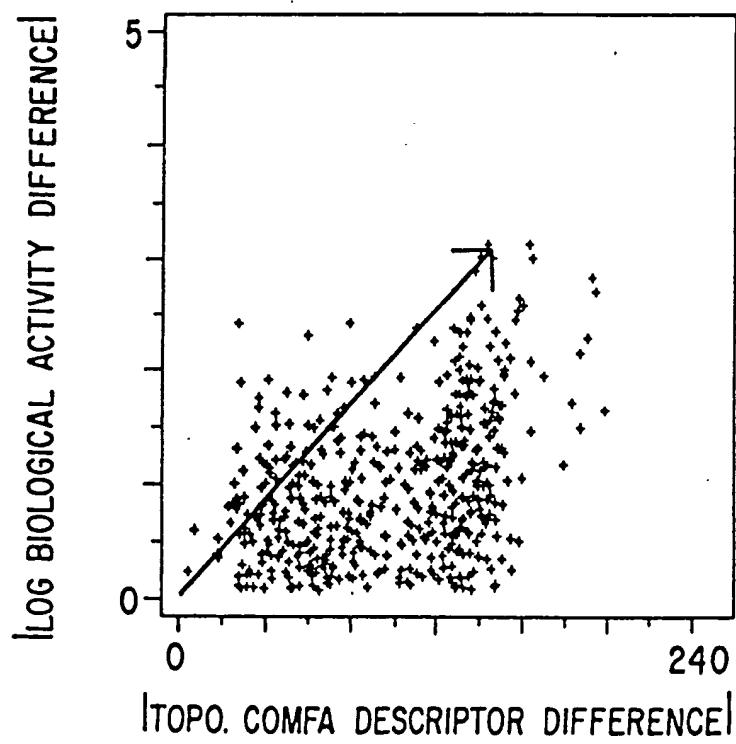


FIG.10(b)

09256344 00206304

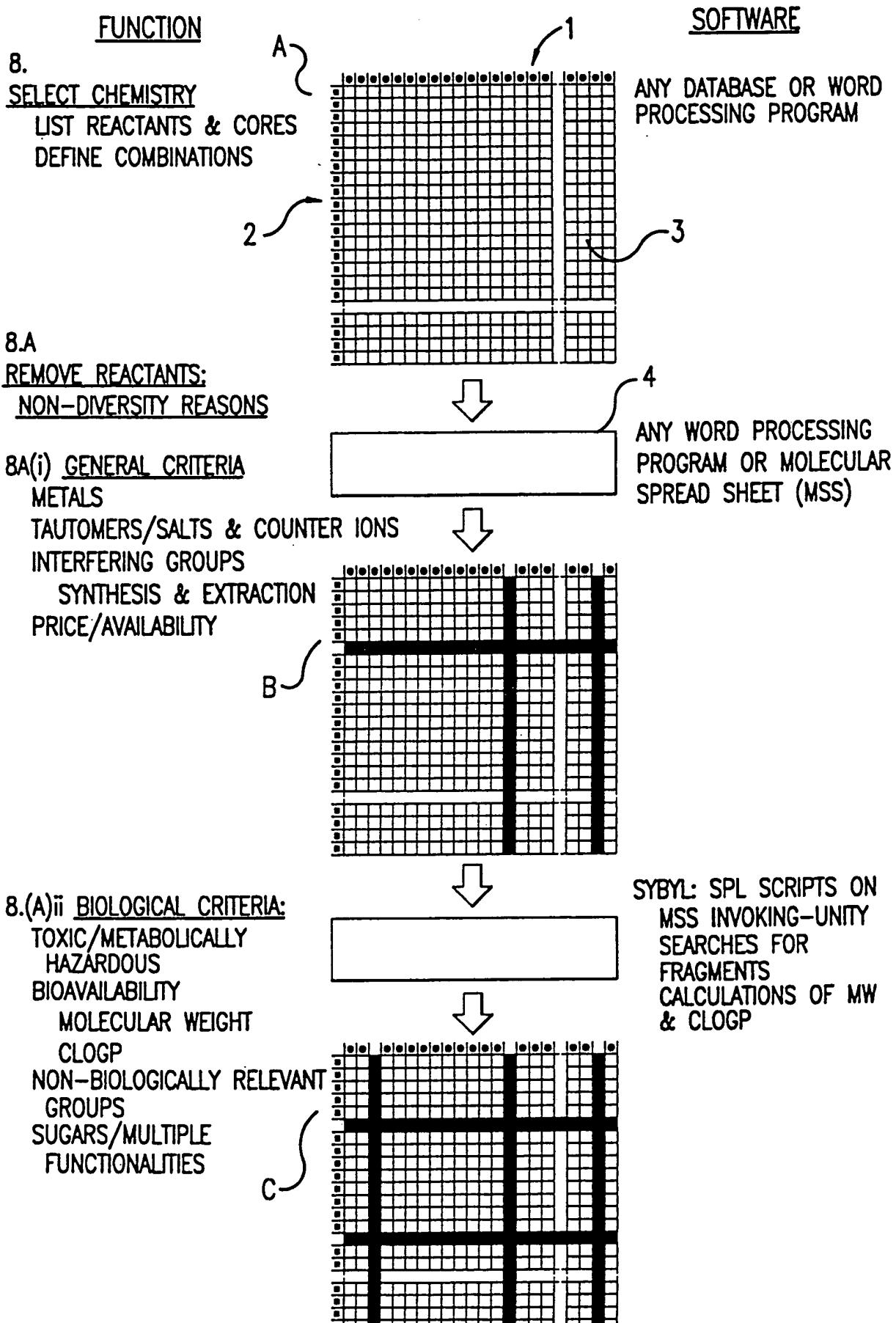


FIG.11(a)

8D

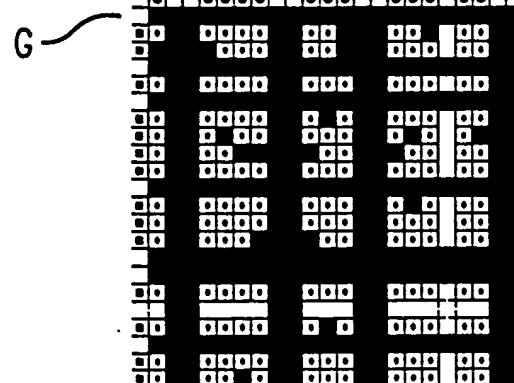
BIOLOGICAL CRITERIA:

METABOLICALLY HAZARDOUS

BIOAVAILABILITY

MOLECULAR WEIGHT

CLOGP



SYBYL: SPL SCRIPTS ON
MSS INVOKING -
UNITY SEARCHES FOR
FRAGMENTS
CALCULATIONS OF MW
& CLOGP

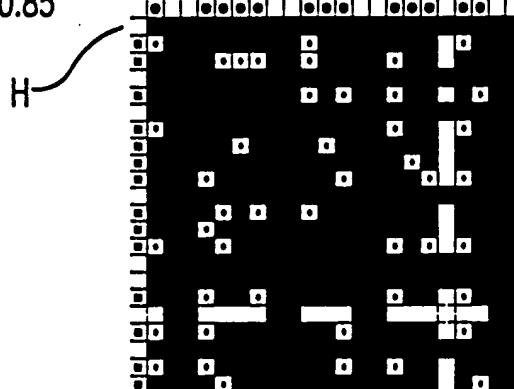
8E

REMOVE NON-DIVERSE
PRODUCTS:

GENERATE TANIMOTO
2D FINGERPRINTS

SAMPLE PRODUCTS:

EXCLUDE TAN \geq 0.85



UNITY

FIG.11(c)

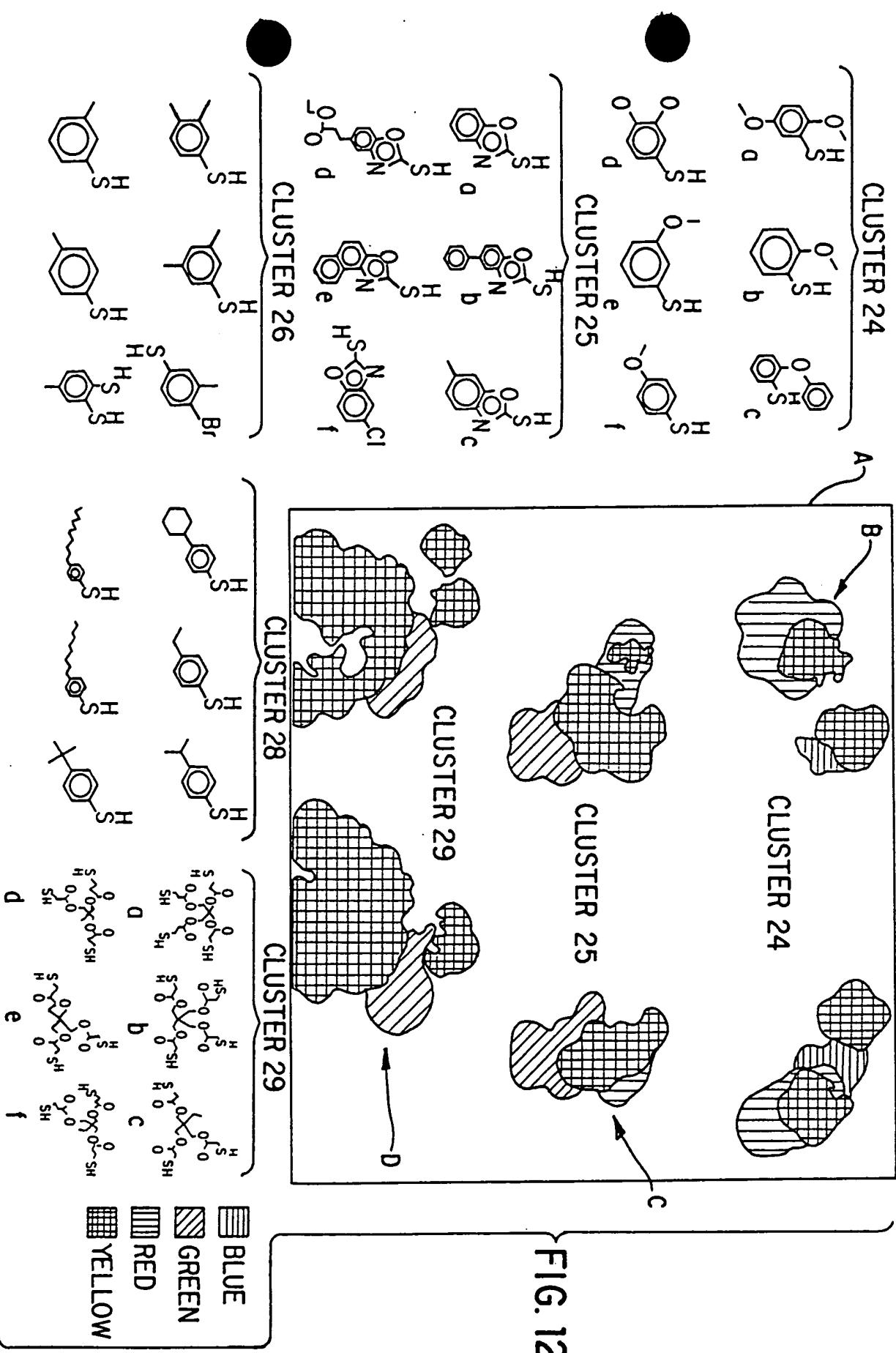
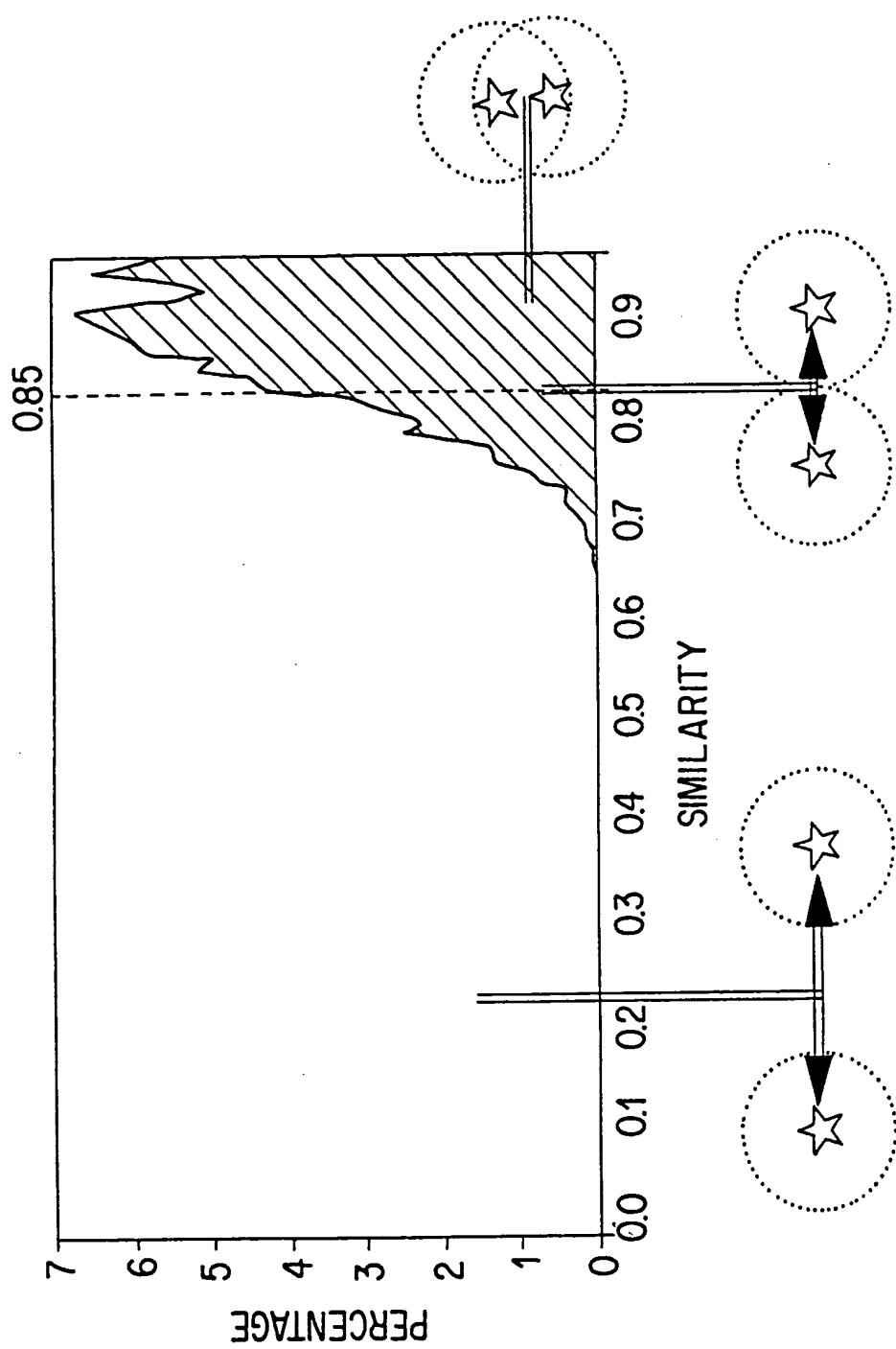


FIG. 12

FIG. 13



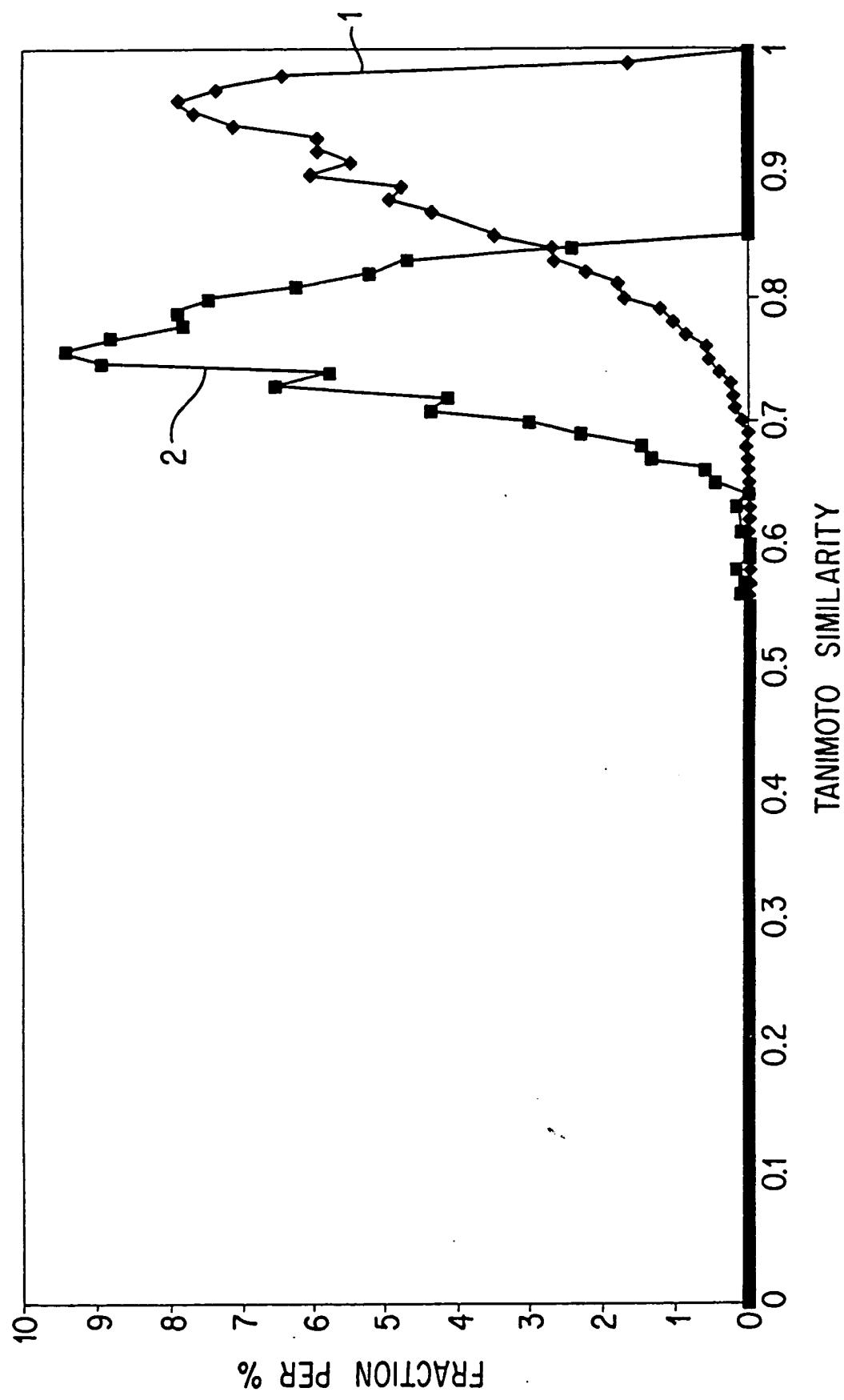


FIG. 14

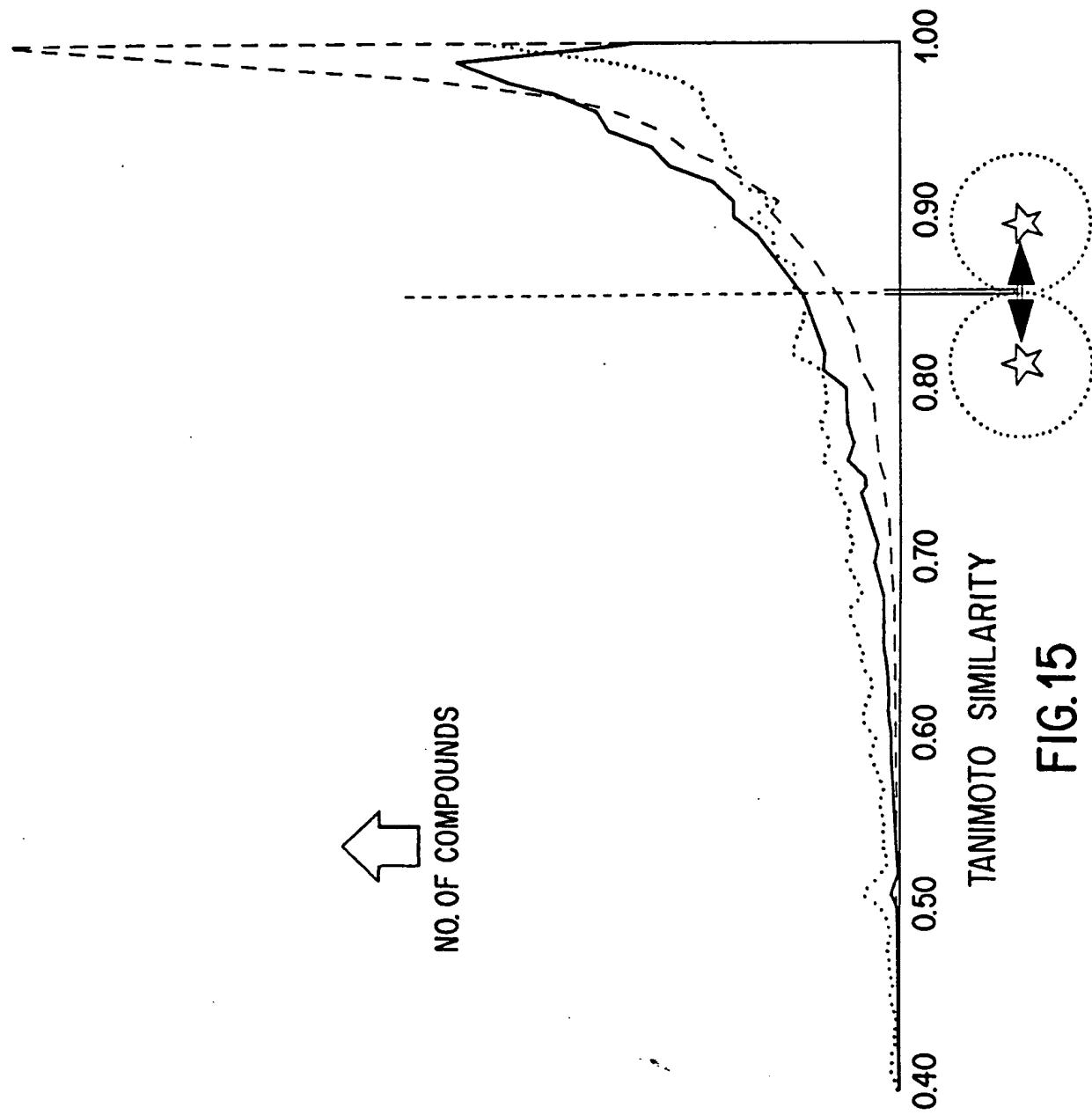


FIG. 15